The GEO-SEQ Project
Quarterly Status and Cost Report
December 1, 2000 – February 28, 2001

Project Overview:

The purpose of the GEO-SEQ project is to establish a public-private R&D partnership that will:

- Lower the cost of geologic sequestration by
  (1) Developing innovative optimization methods for sequestration technologies with collateral economic benefits (such as enhanced oil recovery (EOR), enhanced gas recovery (EGR), and enhanced coalbed methane production), and
  (2) Understanding and optimizing trade-offs between CO_2 separation and capture costs, compression and transportation costs, and geologic sequestration alternatives.

- Lower the risk of geologic sequestration by
  (1) Providing the information needed to select sites for safe and effective sequestration
  (2) Increasing confidence in the effectiveness and safety of sequestration through identifying and demonstrating cost-effective monitoring technologies, and
  (3) Improving performance-assessment methods to predict and verify that long-term sequestration practices are safe, effective, and do not introduce any unintended environmental effects.

- Decrease the time to implementation of geologic sequestration by
  (1) Pursuing early opportunities for pilot tests with our private sector partners and
  (2) Gaining public acceptance.

Technical work began in May 2000 with an initial focus on four tasks: (A) development of sequestration co-optimization methods for EOR, depleted gas reservoirs, and brine formations; (B) evaluation and demonstration of monitoring technologies for verification, optimization, and safety; (C) enhancement and comparison of computer-simulation models for predicting, assessing and optimizing geologic sequestration in brine, oil and gas, and coalbed methane formations; and (D) improvement of the methodology and information available for capacity assessment of sequestration sites. Work continued on these four tasks during the third quarter. Technical progress and accomplishments are discussed below.

Highlights:

- The Tough2 reservoir simulation was enhanced through addition of a module that calculates real gas-compressibility Z factors and fugacities for gaseous mixtures of water, CO_2, and CH_4 using either Peng-Robinson, Redlick-Kwong, or Soave-Redlich-Kwong equations of state.
- Reaction-progress-chemical thermodynamic and kinetic simulations show that minerals such as dawsonite, which might otherwise not be considered, may prove to be important in sequestration of CO_2. Simulations also show that mineral-trapping phases will evolve in the long term as fluid chemistry changes.

- The interplay of heterogeneity, gravity, and fluid properties has significant impact on the capacity of reservoirs to store CO_2. Simulations of carbon sequestration with enhanced gas recovery show that permeability heterogeneity can either enhance or diminish early breakthrough of CO_2.
- Investigations of one of the isotopic tracers for monitoring reservoir processes have focussed on the study of stable-isotope partitioning between CO_2 and representative geologic materials. Results indicated that hydrocarbons and clay have a profound effect on isotopic compositions.
- As a result of a regional survey, a site in Baytown, Texas was chosen as the basis for a realistic numerical simulation of the injection of CO_2 from a power plant into a brine formation. The modeling is focusing in part on the effects of lithologic heterogeneity on CO_2 movement.

Papers Published and Presented:

Johnson, J.W., Steefel, C.I., and Nitao, J.J., Reactive transport modeling of subsurface CO_2 sequestration to identify optimal target formations: Quantifying the relative effectiveness of migration and sequestration processes as a function of reservoir properties, American Geophysical Union Meeting - San Francisco, CA, Fall 2000.

Knox, P.R., and Hovorka, S.D., Geological sequestration of green house gases: Opportunities for Industry-Academe research partnerships, Houston Geological Society Bulletin, 26-33, Fig. 2, January 2001

Oldenburg, C.M., Pruess, K., and Benson, S.M., Process modeling of CO_2 injection into natural gas reservoirs for carbon sequestration and enhanced gas recovery, Energy and Fuels, 15, 293-298, 2001.

Pruess, K., Xu, T., Apps, J., and Garcia, J., Numerical modeling of aquifer disposal of CO_2, Paper SPE-66537, submitted to SPE and presented at SPE/EPA/DOE Exploration and Production Environmental Conference, San Antonio, TX, February 2001.

Outreach Activities

On December 19, 2000, the first Advisory Council Meeting for the GEO-SEQ Project was held at Lawrence Berkeley National Laboratory. The Advisory Council was established to provide input on Project objectives, practicality of approaches, and applicability of results with a focus on rapid technology transfer. Membership reaches beyond immediate partners to ensure broad stakeholder input and wide dissemination of results. The first meeting was held at the end of the first quarter of technical work, thereby providing the Council with a clear picture of the initial focus of the Project activities. At the same time, it was an opportunity to provide early input to the Project.

Attendees at the December 14th meeting were:

Advisory Council Members –

James Clark, Dupont
John Davidson, IEA Greenhouse Gas R & D Program
John Mansoori, BP Amoco
Bob Mc Callister, Exxon
Richard Rhudy, EPRI
Jeff Woliver, Texaco Exploration and Production, Inc.
Nick Woodward, US Department of Energy Office of Science

GEO-SEQ Team Members –

Sally Benson, Lawrence Berkeley National Laboratory (LBNL)
Bob Burruss, United States Geological Survey (USGS)
Charlie Byrer, National Energy Technology Laboratory (NETL)
Dave Cole, Oak Ridge National laboratory (ORNL)
Bill Gunter, Alberta Research Council (ARC)
Susan Havorka, University of Texas Bureau of Economic Geology (TBEG)
John Johnson, Lawrence Livermore National Laboratory (LLNL)
Kevin Knauss, LLNL
Tony Kovscek, Stanford University
David Lau, ARC
Ernie Majer, LBNL
Gerry Moline, ORNL
Larry Myer, LBNL
Robin Newmark, LLNL
Curt Oldenburg, LBNL
Karsten Pruess, LBNL
Chin-Fu Tsang, LBNL
Bert van der Meer, NITG-TNO Netherlands

The meeting began with an overview by Charlie Byrer, Program Manager of the US Department of Energy, Fossil Energy, Carbon Sequestration Program (NETL). The GEO-SEQ Project is one project within the Geologic Sequestration program element. Other program elements involve work in terrestrial and ocean sequestration. An overview of the GEO-SEQ Project was given by Sally Benson, Director. Principal investigators then described the objectives, approaches, and results to date in the nine subtasks which constitute the Project. Copies of the presentations were distributed to the attendees.

The Advisory Council was strongly supportive of the overall GEO-SEQ Project objectives as well as the technical approach being taken in each subtask. The Council endorsed the multidisciplinary approach being taken by the Project. While noting that scoping studies are initially needed, the Council recommended that focus be put on specific technologies as soon as possible, an approach consistent with the GEO-SEQ program plan. The Council strongly encouraged continued close interaction with industry, particularly in selecting field test sites and carrying out work at these sites. Oil and gas fields continue to be the strongest candidates, though other opportunities (for example, those related to deep injection of hazardous waste) were also discussed.

Subtask-specific recommendations included the following:

- Development of criteria for selection of reservoirs for co-optimizing CO_2 sequestration and EOR can benefit from numerous CO_2 EOR case histories.
- Modeling of enhanced gas recovery using CO_2 should continue with realistic well spacing and study of the effects of solubility.
- The possibility of injecting CO_2 into a gas condensates reservoir could be investigated.
- Geochemical modeling should be supported by experimental studies.
- Caprock integrity should be addressed in monitoring studies.
- Time-lapse techniques are important components of a monitoring strategy.
- Focus on development of optimized monitoring techniques.
- Stress-dependent effects need to be incorporated in coal-bed methane models.
- While an open code comparison is supported, it would also be advantageous to identify incentives for participation of for-profit companies.

Task Summaries

Task A: Develop Sequestration Co-Optimization Methods

Subtask A-1: Co-optimization of carbon sequestration and EOR and EGR from oil reservoirs.

Accomplishments:

- The interplay of heterogeneity, gravity, and fluid properties are shown to have significant impact on capacity of oil reservoirs to store CO_2.

Summary:

The objectives of this subtask are (1) to assess the feasibility of co-optimization of CO_2 sequestration and EOR and (2) to develop techniques for selecting the optimum gas composition for injection. Results will lay the groundwork necessary for rapidly evaluating the performance of candidate sequestration sites as well as monitoring the performance of CO_2 EOR.

The initial focus has been to assess the feasibility of CO_2 sequestration in depleted or inactive oil reservoirs. Existing CO_2–EOR selection criteria have been examined in light of the need to maximize CO_2 storage in a reservoir and new criteria developed.

Progress This Quarter: Work continued on a report discussing the screening criteria established for combined EOR and sequestration. Work also was initiated on surveying the number and location of current and abandoned oil fields that meet this criterion.

Work Next Quarter: The report "Criteria for Selecting Oil Reservoirs Suitable for CO_2 Sequestration" will be completed and circulated for comments. Work will continue on an operational model for simultaneous EOR and sequestration that maximizes ultimate oil recovery and placement of CO_2 into oil reservoirs for carbon sequestration.

Subtask A-2: Feasibility assessment of carbon sequestration with enhanced gas recovery (CSEGR) in depleted gas reservoirs.

Accomplishments:

- The Tough2 reservoir simulation was enhanced through addition of a module that calculates real gas compressibility Z factors and fugacities for gaseous mixtures of water, CO_2, and Ch_4 using either Peng-Robinson, Redlick-Kwong or Soave-Redlich-Kwong equations of state.

Summary:

The objectives of this subtask are to assess the feasibility of injecting CO_2 into depleted natural gas reservoirs for (1) sequestering carbon and (2) enhancing methane (CH_4) recovery. Investigation will include assessments of (1) CO_2 and CH_4 flow and transport processes, (2) injection strategies that retard mixing, (3) novel approaches to inhibit mixing, and (4) identification of candidate sites for a pilot study.

Feasibility is being assessed through numerical simulation of CO_2 injection into a model system based on the Rio Vista gas field in California. Positive results of this assessment have led to scoping studies for a CSEGR pilot.

Progress this Quarter: The expected processes and needs for a CSEGR pilot study have been outlined. Among the expected processes are gas mixing and its potential enhancement resulting from heterogeneity. Figure 1 presents a representative heterogeneous-permeability field generated for simulating gas flow with heterogeneity. Figure 2 shows the corresponding gas flow field and CO_2 mass fraction in the gas phase. Depending on the heterogeneity structure, permeability heterogeneity can either enhance or diminish early breakthrough of CO_2.

Development of simulation capabilities was continued by incorporating into the TOUGH simulator a new real gas properties module that will allow simulations at pressures above the critical pressure for CO_2 (74 bars). This module calculates real-gas-compressibility Z factors and fugacities for gaseous mixtures of water, carbon dioxide, and methane using either Peng-Robinson, Redlich-Kwong, or Soave-Redlich-Kwong equations of state. The NIST14 database for testing against the newly developed gas properties module was also obtained. NIST14 does not include water as a component in the mixture, whereas the new module does.

Initial contacts have been made with California gas field operators to discuss a CSEGR pilot.

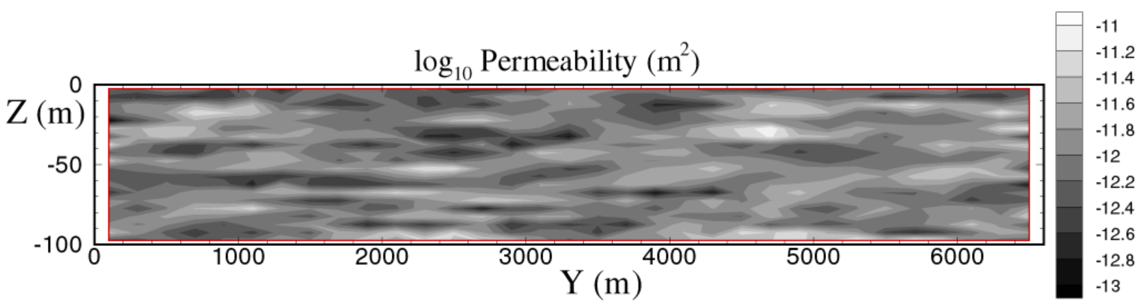

Figure 1. Representative heterogeneous permeability field.

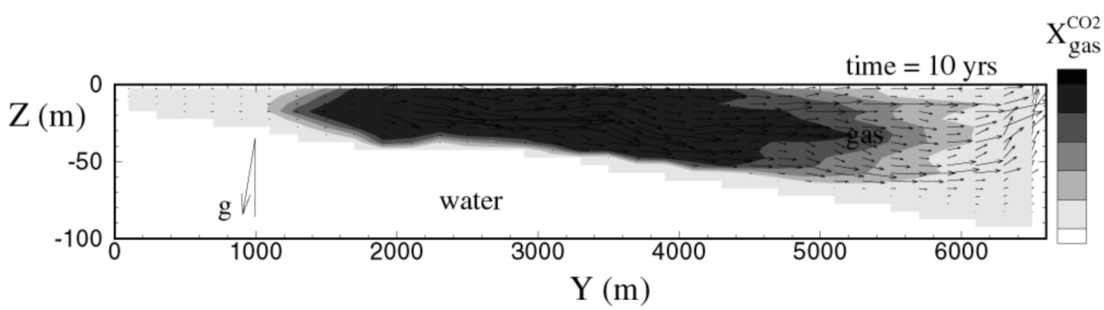

Figure 2. CO_2 mass fraction in the gas and gas velocity vectors after 10 years of CO_2 injection into heterogeneous reservoir.

Work Next Quarter: The new gas properties module will be tested and validated, including comparison with the NIST14 database. Simulation studies involving higher reservoir pressures will begin. Discussions with California gas field operators on possible CSEGR pilot studies will continue.

Subtask A-3: Evaluation of the impact of CO_2 aqueous fluid and reservoir rock interactions on the geologic sequestration of CO_2, with special emphasis on economic implications.

Accomplishments:

- Reaction-progress-chemical thermodynamic and kinetic simulations show that minerals such as dawsonite, which might otherwise not be considered, may prove to be important in sequestration of CO_2. Simulations also show that mineral trapping phases will evolve in the long term as fluid chemistry changes.

Summary:

Numerical simulations are being carried out to evaluate geochemical changes accompanying injection of a waste stream containing SO_2, NO_2 and H_2S. Simulations are equivalent to batch-type (closed system) reactions including full-dissolution kinetics (including acid catalysis) for all of the mineral phases present in the reservoir rock. A rock composition is used with modal abundances appropriate for a feldspathic-sandstone reservoir (containing clay and carbonate with and without a Fe-bearing phase), and a carbonate reservoir (comprised of calcite, dolomite, and siderite).

Progress This Quarter: Additional simulations were carried out for evaluation of the impact of SO_2, NO_2 and H_2S. In one simulation, brine that was initially equilibrated with a gas phase consisting of 80 b CO_2 and 10 b H_2S is allowed to react with the feldspathic sandstone reservoir in isolation from the gas phase. Note that this high H_2S fugacity is not unlike that present in a waste stream produced in a coal gasification process. In this simulation it was assumed that (in the short-term) redox disequilibria will pertain, so that effectively, all redox reactions are turned off. This means, for example, that dissolved H_2S remains H_2S and does not oxidize to SO_4^{2-}. The initial fO_2, while low (log FO_2 = -55, approximately equivalent to initial buffering by hematite-siderite), is still just high enough that at redox equilibrium all the H_2S would convert to SO_4^{2-}. The results after 30 years of reaction are presented in Figure 3, while the results after continued reaction in the same system after 500 years are presented in Figure 4.

Notice that in this simulation (Figure 3) the reservoir rock carbonate minerals (calcite and siderite) react rather quickly with the dissolved CO_2, raising the pH until the carbonate minerals are essentially equilibrated with the resulting solution. The existing carbonate minerals are not sequestering the CO_2 in this case. The only form of sequestration at this point is the CO_2 present in dissolved form in solution. From this point forward in the calculation, the principal reaction involves dissolution of the K-feldspar at the still-slightly-acid pH of approximately 4.8. However, the Al released from the K-feldspar combines with Na from the brine and dissolved CO_2 to form the mixed hydroxycarbonate mineral dawsonite. This new secondary mineral is sequestering CO_2 via mineral trapping. The silica released from the dissolving K-feldspar is precipitated as the silica polymorph chalcedony, as well as producing additional quartz. Notice that the absolute abundance of quartz is so much larger than the other minerals that we have not plotted it. It grows in linearly at a rate determined by its kinetic rate law, increasing in volume from 1804 cm^3 to 1808 cm^3 after 30 years and to 1832 cm^3 after 500 years. The chalcedony and dawsonite both grow at a rate determined by the dissolution rate of the K-feldspar.

The dissolved silica in the simulation (Figure 4) maintains a steady-state concentration reflecting the sum of the processes: K-feldspar dissolution, quartz and chalcedony precipitation. After 10 years or so, the K-feldspar approaches equilibrium with the solution and stops dissolving. After this point, the chalcedony starts dissolving at a rate determined by quartz growth, until after 90 years it is completely consumed. Quartz keeps growing and lowers the dissolved silica to the point that K-feldspar starts dissolving again, allowing more dawsonite to form, sequestering more dissolved CO_2. Note that the pH also increases slightly at the point that the chalcedony disappears, allowing additional calcite to precipitate and also sequestering more dissolved CO_2. By the end of the run at 500 years, quartz is only slightly supersaturated and its rate of growth has slowed considerably. The CO_2 concentration in solution decreases from more than 1.3 m to less than 0.9 m after 500 years.

This simulation illustrates several important points. First, the minerals that may prove important in sequestering CO_2 may not be the obvious ones (i.e., calcite, dolomite, siderite, magnesite and the like). Second, the mineral trapping of CO_2 is a long-term, ongoing process that will evolve as solution chemistry evolves over time and minerals evolve in response to the fluid chemistry changes.

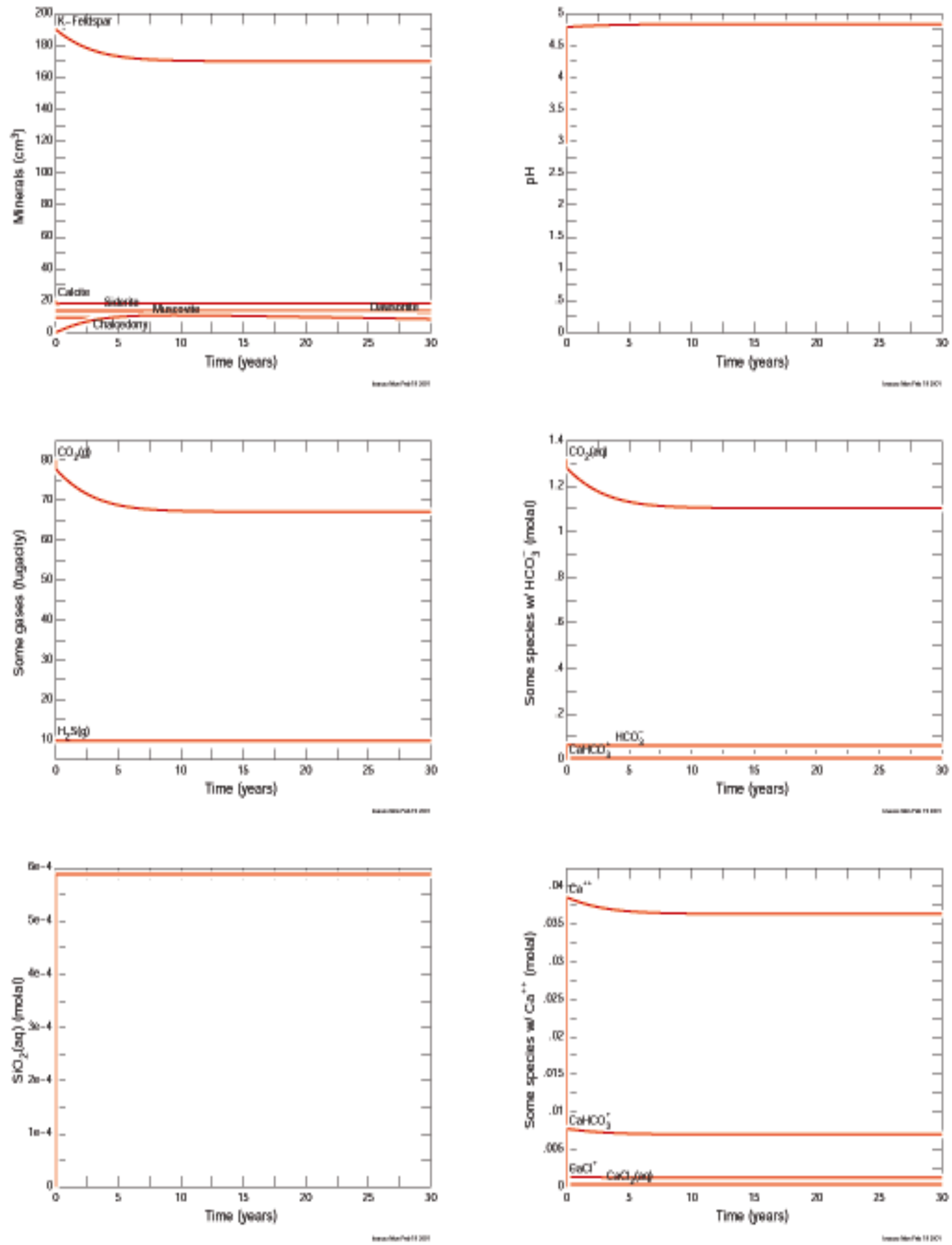

Figure 3. Numerical results after 30 years of reactions.

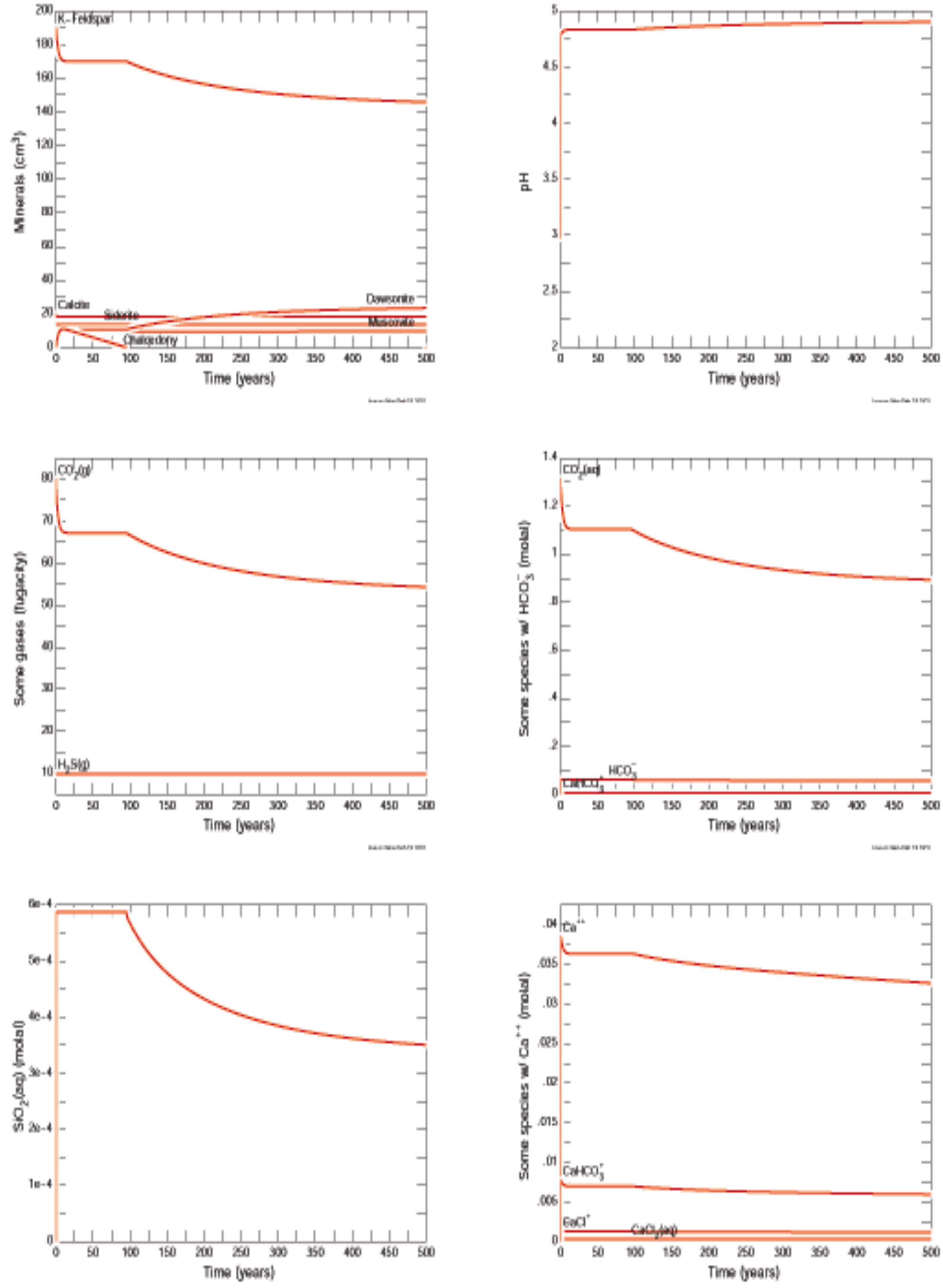

Figure 4. Numerical results after 500 years of reactions.

Work Next Quarter: Investigation of the impact of SO_2, H_2S, and NO_2 in the CO_2 waste stream will continue.

Task B: Evaluate and Demonstrate Monitoring Technologies

Subtask B-1: Sensitivity modeling and optimization of geophysical monitoring technologies

Accomplishments:

- Reservoir stimulations were initiated to predict production and the distribution of fluids in the reservoir resulting from injection of CO_2 at the Chevron Lost Hills field pilot.

Summary:

The objectives of this task are to: (1) demonstrate methodologies for and carry out an assessment of the effectiveness of candidate geophysical monitoring techniques, (2) provide and demonstrate a methodology for designing an optimum monitoring system, and (3) provide and demonstrate methodologies for interpreting geophysical and reservoir data, to obtain high-resolution reservoir images.

The Chevron CO_2 pilot at Lost Hills, California, is being used as an initial test case for developing these methodologies. Work to date has focused on modeling the geophysical response of seismic and electromagnetic (EM) surveys made before injection of CO_2. The first step in this process was to perform a reservoir simulation (provided by Chevron) of fluid production (oil, water, gas) and fluid injection (water flooding) which took place prior to CO_2 injection. The reservoir model simulations provide estimates of porosity, fluid saturation, pressure, and distribution as a function of lithology in the reservoir. Using well logs and rock physics models, this information was converted to seismic velocities and electrical conductivity. Forward simulations were then performed to generate the seismic wavefield that would be sampled by a crosswell seismic survey and the electrical field that would be sampled by a crosswell EM survey.

In a parallel effort numerical simulations have also been carried out to access the sensitivity of electrical resistance tomography (ERT) for detection of CO_2. These studies have used models representative of expected conditions at the Hall-Gurny Field, Russell County, Kansas, and the Sleipner project, Norway.

Progress this Quarter: Reservoir simulations were initiated to forward model the CO_2 injection process at the Lost Hills pilot. This involves prediction of fluid production (oil, gas, and brine) as well as injection of CO_2 Results will be used as input to geophysical simulations, which will model the post-CO_2 injection crosswell seismic and crosswell EM surveys.

Work Next Quarter: Results of reservoir simulation runs for CO_2 injection will be converted to electrical resistivity and velocity and used to compute the expected geophysical responses. A 3-D velocity model with an orbital vibrator source will be simulated. The computed responses will be compared to the observed data and used to update both the geologic and petrophysical models to improve the fit between observed and calculated data. Work will also continue on investigating the potential for using ERT, with a focus on finding a site for a field test.

Subtask B-2: **Field data acquisition for CO_2 monitoring using geophysical methods**

Accomplishments:

- Processing was begun of the results from an innovative single well seismic survey. The survey, which will be repeated after CO_2 injection, fills a gap in scales between sonic logging and surface seismic.

Summary:

The goal of this subtask is to demonstrate (through field-testing) the applicability of single-well, crosswell, surface-to-borehole seismic, crosswell electromagnetic (EM), and electrical-resistance tomography (ERT) methods for subsurface imaging of CO_2.

The CO_2 injection pilot operated by Chevron USA in Lost Hills, California, provides an early opportunity to test these techniques. This pilot is divided into four injection-centered, 2.5-acre patterns as shown in Figure 5. The figure also provides some interpreted geology for the site. The production interval is from 1,200 feet to 2,100 feet below ground surface, and the CO_2 injection interval is from 1,500 feet to 2,000 feet. The CO_2 injection began in August 2000 at a relatively low flow rate of 125 million cubic feet (Mcf) per day and was gradually increased to 425 Mcf/day per injection well. The injection pressure is being held at 800–900 psi and the reservoir temperature is about 100 F. At these pressure and temperature conditions the CO_2 is expected to be in gas phase. In early January 2001, CO_2 injection was stopped in the four injection wells because of sanding problems in some of the producing wells. The wells were cleaned out, and CO_2 injection has been restarted in one of the injection wells.

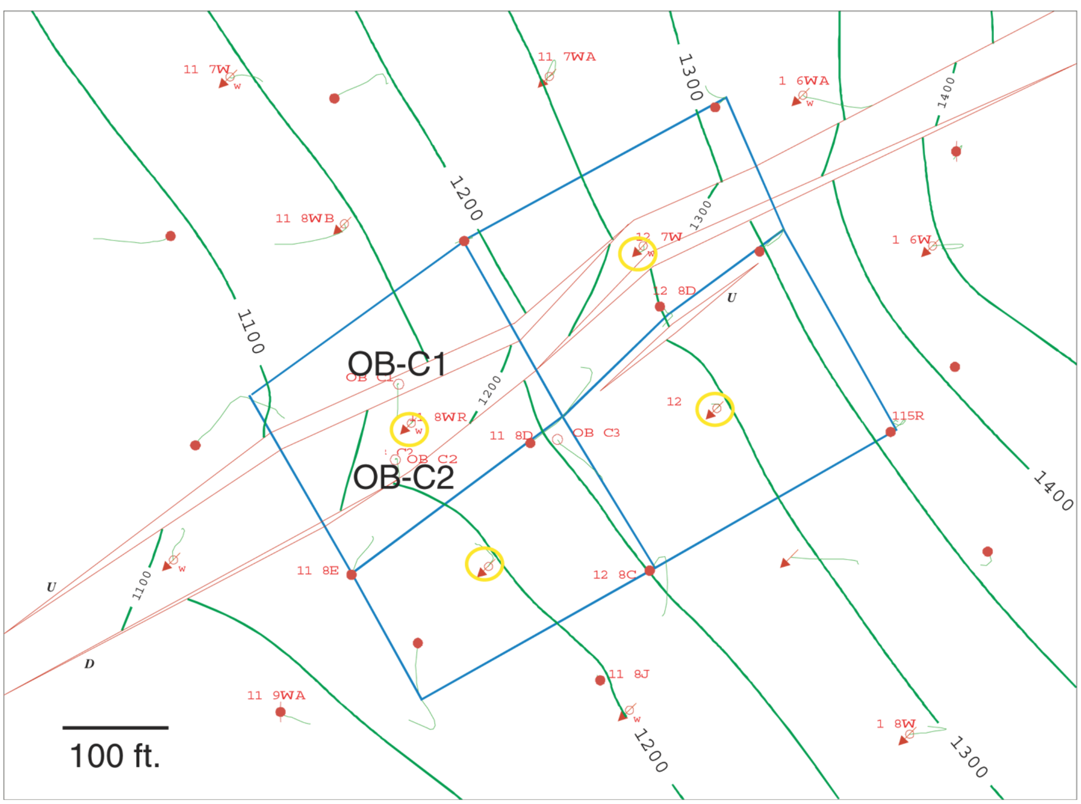

Figure 5. CO_2 injection site (blue lines) with contoured top of reservoir (green lines) and interpreted faults (red lines).

The reservoir volume around Injection Well 11-8WR is being monitored by high-resolution geophysical techniques. During the first quarter, crosswell seismic and EM measurements were made between observation wells OB-C1 and OB-C2 and single-well seismic measurements were made in OB-C1. During the second quarter, preliminary tomographic images of velocity and electrical conductivity were obtained.

Progress this Quarter: Analysis of the results of the single well seismic imaging (SWSI) survey performed in OB-C1 was begun. A SWSI survey is an innovative procedure designed to improve near-borehole imaging and fill the gap in scales of subsurface imaging between sonic logging and crosswell surveys. Figure 6 shows a schematic representation of a SWSI survey as compared to sonic logging. The SWSI survey uses a seismic source and a string of sensors at a relatively large offset from the source to sample a volume around the borehole of tens of cubic meters. As shown in Figure 6, a SWSI survey can be used for reflection imaging of a vertical discontinuity such as a fracture zone. In particular, a gas filled fracture zone is an ideal target for SWSI imaging. Therefore, we are hopeful that the CO_2 injection interval at Lost Hills (with presumed gas phase CO_2) will be imaged by our SWSI survey.

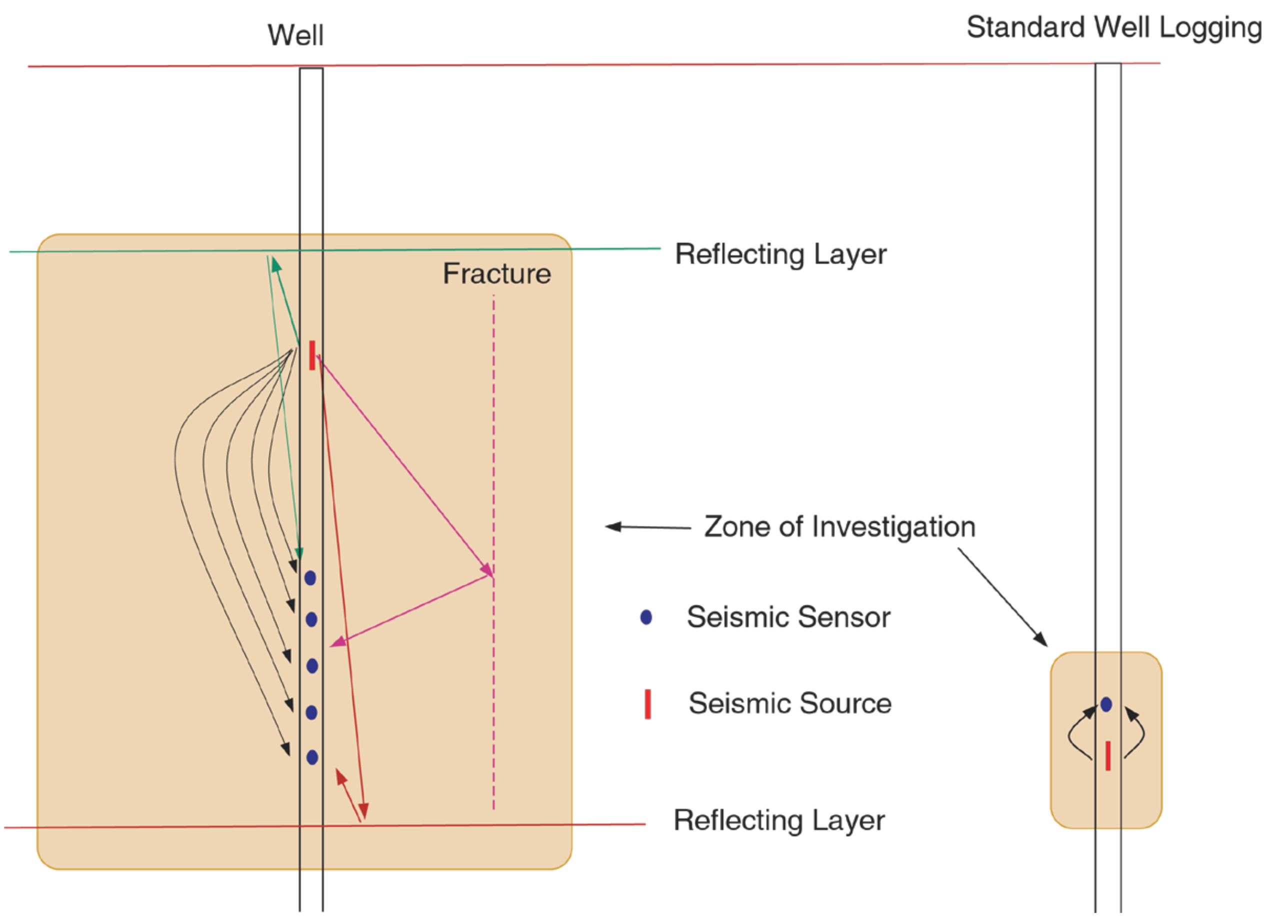

Figure 6. Schematic representation of single well seismic imaging (SWSI) system.

The August 2000 SWSI acquisition used LBNL's piezoelectric source and string of 15 borehole hydrophones. The source signal was a pulse giving about 500–3500 Hz bandwidth. The source offset was 7.4 m and the sensor spacing was 1.524 m for each of 15 sensors. A source-monitor accelerometer was also recorded for each shot. Each recorded shot was a stack of 25 pulses of the source, recorded for 250 ms, at a sample rate of 0.125 ms. Shots were recorded every 2 feet (0.61 m) for source depths from 2,020 feet to 1,500 feet (616 to 457 m). An additional SWSI test was performed using three-component geophone sensors between depths 1,850 and 1,550 feet (564 to 472 m).

Figure 7 shows a typical shot gather. Electrical cross talk from the high voltage (4 kV) piezoelectric source is at zero time, while the P-wave arrives between 7 and 20 ms. The slower tube-wave (a type of borehole surface wave) arrives following the P-wave. Because of the high-amplitude noise of the tube wave, we use the time window between the P-wave and the tube wave for imaging features surrounding the borehole. Figure 8a and 8b show data gathers for a single hydrophone offset 34 and 64 feet (10.4 and 19.5 m) respectively below the source. In this data gather, the variation in arrival times as a function of depth can be seen, as well as changes in the "coda" of energy arriving between the P-wave and tube-wave. The variation of P-wave arrival time will be used for identifying near-borehole changes in material property (similar to a sonic log, but with larger radius of investigation). Changes in the coda will be used to identify regions of increased reflectivity from which we will infer the presence of CO_2. Ideally, a coherent reflection will be seen in the code that can be imaged with CDP techniques.

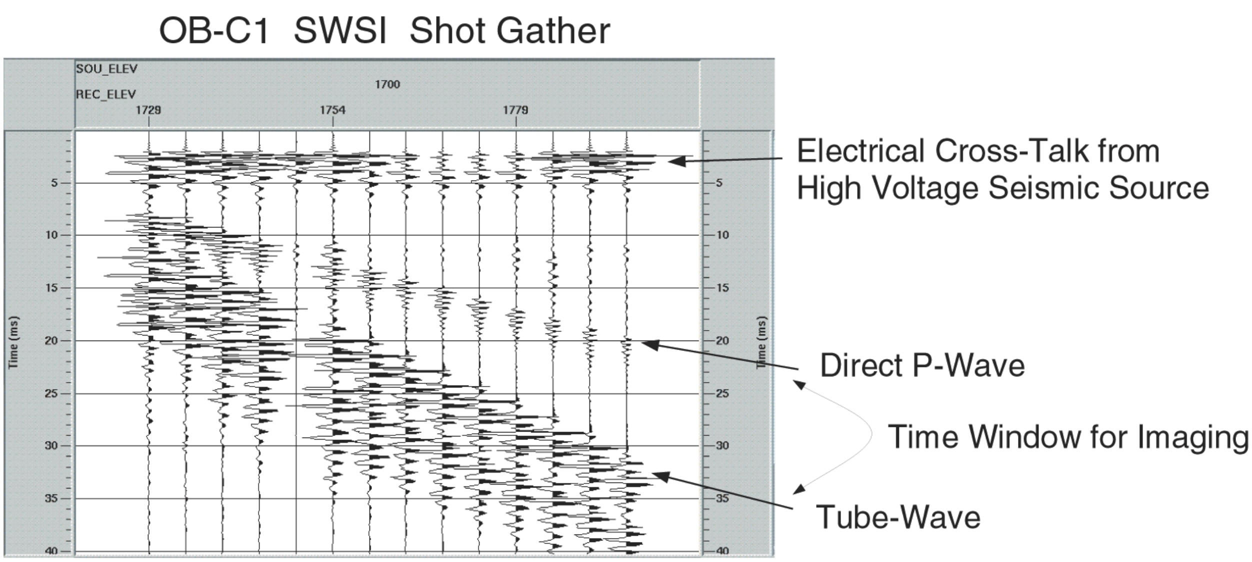

Figure 7. Example of SWSI shot gather.

Work Next Quarter: Processing, modeling, inversion, and interpretation of the crosswell seismic and EM data sets will continue. Preparations will be made for the post-injection time-lapse surveys, which are expected to take place in late May.

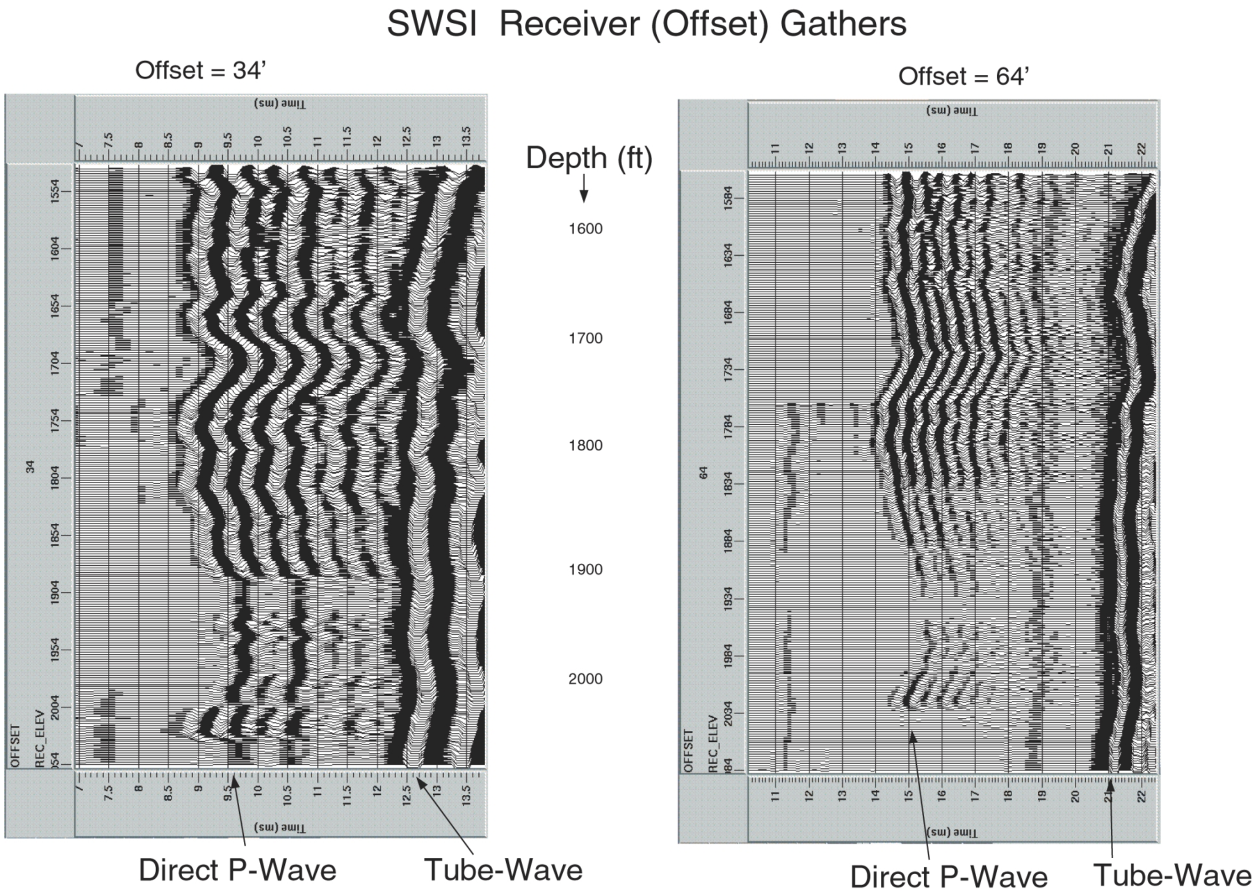

Figure 8. Examples for receiver, gathers for hydroplane, offsets of 34 feet and 64 feet.

Subtask B-3: Application of natural and introduced tracers for optimizing value-added sequestration technologies

Accomplishments:

- Investigation of stable isotope partitioning between CO_2 and representative geological materials has indicated that hydrocarbons and clay have a profound effect on isotopic compositions.
- Characterization of a set of standard coal samples was carried out in preparation for CO_2 – CH_4 sorption-desorption and isotope partitioning experiments.

Summary:

The overall goal of this effort is to provide methods that utilize the power of natural and introduced tracers to decipher the fate and transport of CO_2 injected into the subsurface. The resulting data will be used to calibrate and validate predictive models used for (1) estimating CO_2 residence time, reservoir storage capacity, and storage mechanisms; (2) testing injection scenarios for process optimization; and (3) assessing the potential leakage of CO_2 from the reservoir.

To date work has focused primarily on isotopic tracers. Effort has been directed to accessing carbon and oxygen isotope change as the CO_2 reacts with potential reservoir phases. In addition to investigation of generic core fluid systems, studies have also been carried out using core from the Chevron Lost Hills CO_2 pilot. Last quarter model calculations showed that carbon isotope values of CO_2 become less negative through reactions with aqueous HCO_3, calcite, or hydrocarbon rich rock from the Lost Hills reservoir.

Progress this Quarter: Efforts this quarter have focused primarily on the isotopic tracer work. The carbon and oxygen isotope partitioning has been measured between CO_2 and a variety of geological materials at 25°C. In a continuation of our previous effort involving organic-rich diatomaceous core from the Lost Hills reservoir, we expanded the types of geological materials to include quartz, calcite and montmorillonite. We also examined the isotope partitioning between CO_2 and crude oil provided by Chevron from Lost Hills. The focus here was to demonstrate whether isotopic behavior was reproducible and reversible, and to assess the impact hydrocarbons have on the isotopic behavior. To accomplish this, we used isotopically different CO_2 gases ($\delta^{13}C$ = + 50.4 vs -40.7$^0/_{00}$; $\delta^{18}O$ = -13.5 versus –17.5$^0/_{00}$), reacting with these materials for different lengths of time (3, 5, and 7 days) at slightly different PCO_2 levels (0.003 to 0.0055 MPa). Steady state partitioning for both carbon and oxygen isotopes was generally reached after 5 days. In all cases, the free CO_2 was isotopically enriched in ^{13}C and ^{18}O relative to gas sorbed onto the solids. The magnitude of the partitioning for oxygen always exceeded that of carbon by roughly a factor of 2–3. The carbon isotope partitioning was greatest between CO_2 and the oil (7-10$^0/_{00}$) followed in order by montmorillonite (7-8$^0/_{00}$), Lost Hills core (4-7$^0/_{00}$), calcite (2-3$^0/_{00}$), and finally quartz (1-2$^0/_{00}$). The order of partitioning was somewhat different for oxygen isotopes: greatest in the Lost Hills core (20-35$^0/_{00}$), followed by montmorillonite (22-27$^0/_{00}$), Lost Hills crude oil (7-13$^0/_{00}$), calcite (6-12$^0/_{00}$), and finally quartz (2-3$^0/_{00}$;). These preliminary results clearly indicate that hydrocarbons and clay may have a profound effect on isotope compositions of CO_2 injected into the subsurface.

Four Argon Premium coal samples have been obtained for use in both CO_2-CH_4 sorption-desorption and isotope-partitioning experiments. These four coals are a medium-volatile bituminous (#1, Upper Freeport seam, PA), a sub-bituminous (#2, Wyodak-Anderson seam, WY), a low volatile bituminous (#5, Pocahontas No. 3 seam, VA), and a high volatile bituminous (#7, Lewiston-Stockton seam, WV). Tests completed to date include scanning electron microscopy (SEM), grain size analysis, and N_2 BET surface area measurements.

Work Next Quarter: Efforts in the next quarter will focus on four main areas:

a) Continuation of core-gas-fluid isotope exchange experiments, emphasizing the Lost Hill samples, more generic minerals representative of common reservoir lithologies, such as quartz (sandstone analogue), calcite (limestone analogue), and montmorillonite (mudstone analogue) and the Argon Premium coal samples.
b) Initiate CO_2- CH_4 sorption-desorption experiments using Argon Premium coals as well as Lost Hills core and mineral end-members, quartz, calcite, and montmorillonite.
c) Initiate a modeling effort using Geochemists Workbench to assess the magnitude of carbon and oxygen isotope partitioning during gas-brine-mineral reactions relevant to subsurface aquifer formation conditions.
d) Complete construction of flow-through column apparatus and initiate laboratory testing of the applied tracers using the same geological materials as in the isotopic tracer experiments.

Task C: Enhance and Compare Simulation Models

Subtask C-1: Enhancement of numerical simulators for greenhouse gas sequestration in deep, unmineable coal seams.

Accomplishments:

- Testing of two sets of numerical simulation problems using BP-Amoco's GCOMP and CSIRO's SIMED II was completed.
- The CBM numerical simulator, ECLIPSE, was evaluated in cooperation with software developers at Schlumberger GeoQuest.
- The first benchmark problem sets were posted on the ARC website.

Summary:

The goal of this subtask is to improve simulation models for capacity and performance assessment of CO_2 sequestration in deep, unmineable coal seams.

Work began with definition of the physical processes that ultimately should be included in coalbed methane (CBM) numerical simulators. Benchmark problems were then developed for testing and comparison of available CBM codes. The first problems set is a single-well test with CO_2 injection into a coal seam. The second set is an enhanced coalbed methane (ECBM) process with CO_2 injection in a 5-spot well pattern. A website was established to document the benchmark problems and to post solutions. In the second quarter, testing of the first two problem sets was completed using the simulators STARS and GEM.

Progress This Quarter: Testing and comparison of available CBM simulators continued. Two benchmark problems, which have been posted on the ACR website, are run on each simulator. This quarter, testing using the BP-Amoco simulator GCOMP and the CSIRO simulator SIMED II was completed and work began using the Schlumberger GeoQuest simulator ECLIPSE.

In a parallel effort, work was started on establishing the feasibility of developing analytic solutions for multicomponent gas flow coupled with absorption in coalbeds.

Work Next Quarter:

- Complete testing of the first two problem sets using Schlumberger GeoQuest ECLIPSE.
- Complete the report entitled "Modeling of Carbon Dioxide in Coalbed: Model Improvement", by David H.-S. Law, W.D. (Bill) Gunter and L.H.G. (Bert) van deer Meer.
- More complex problem sets in which several important mechanisms such as mixed gas diffusion (using dual porosity model) and coal shrinkage/swelling will be developed.

Subtask C-2: Intercomparison of reservoir simulation models for oil, gas, and brine formations

Accomplishments:

- Commitments for participation in a code intercomparison study for CO_2 sequestration in oil, gas, and brine formations were received from ten groups in six countries.
- The intercomparison study materials were placed on the GEO-SEQ website.

Summary:

The objective of this subtask is to stimulate the development of models for predicting, optimizing, and verifying CO_2 sequestration in oil, gas, and brine formations. The approach involves: (1) developing a set of benchmark problems, (2) soliciting and obtaining solutions for these problems, (3) holding workshops of industrial, academic, and laboratory researchers, and (4) publishing results.

To date, a set of light benchmark problems have been established. Processes encompassed by these problems include carbon sequestration with enhanced gas recovery, aquifer disposal of CO_2 (with geochemical interactions), hydro-mechanical coupled processes, and miscible and inmiscible displacement of oil by CO_2.

Progress this Quarter: The materials for the CO_2 code intercomparison study were finalized, mailed out, and posted on the web. This includes a "First Announcement and Call for Participation" as well as a detailed report on design and milestones of the study, and specifications of a first set of eight test problems.

Work Next Quarter: We will perform simulation studies of test problems for the code intercomparison and begin to develop enhanced and more realistic problem specifications. We will also continue to interact with the various participating groups, providing guidance and commenting on preliminary results.

Task D: Improve the Methodology and Information for Capacity Assessment

Accomplishments:

- A site for modeling a realistic injection of CO_2 from a power plant into a brine formation was defined, modeling parameters selected, and an initial simulation run to model the impact of lithologic heterogeneities on the CO_2 plume.

Summary:

The objectives of this task are to: (1) improve the methodology and information available for assessing the capacity of oil, gas, brine, and unmineable coal formations; and (2) provide realistic and quantitative data for construction of computer simulations that will provide more reliable sequestration capacity estimates.

As a first step in performing capacity-assessment simulations in brine formations, mathematical models were developed to assess the relative contributions to total sequestration capacity from CO_2 (1) in the gas phase, (2) dissolved in the aqueous phase, and (3) in solid minerals. Capacity factors for the three different storage modes were defined as the equivalent gas saturations that would be required to store the same amount of CO_2. These capacity factors were partially evaluated through analytical estimates and numerical simulations.

The Texas Gulf coast was targeted as an area from which a realistic data set could be generated for use in simulation of capacity in brine formation. Location and identifying information were compiled for large industrial CO_2 emitters, and geologic data for the Frio and Oakville reservoirs was compiled.

<u>Progress this Quarter</u>: A realistic scenario for CO_2 injection into a brine formation was designed. As a result of a regional survey (www.beg.utexas.edu/co2), we selected for our investigation an injection site in Baytown, Texas that is representative of an area for both high CO_2 emissions and high-quality and well-characterized subsurface conditions for geologic sequestration. This is also an area for public concern over air quality. The USGS Geode database reports 1997 CO_2 emissions of 4.3 million metric tons of CO_2 for the 2295 MW gas-fired Cedar Bayou power plant, and an unknown additional amount of CO_2 is emitted by the adjacent Bayer Refinery. The top of the selected injection horizon, the uppermost sand of the middle Frio Formation, lies at a depth of 1,850 m. As is typical for a brine-formation injection site, we do not have sufficient well data to map permeability in the injection interval. For this simulation, we therefore selected a geologically constrained probabilistic procedure to create a model grid.

The depositional setting of the selected sand was interpreted from published regional, dip-oriented, well-log cross sections to be deltaic and barrier strandplain systems. We interpreted the depositional facies and the scale of both sandy and muddy depositional features of 10 layers separated by subregionally extensive shales (flooding surfaces) within a one hundred meter thick, sand-rich interval on the basis of a recently completed Burea study of the adjacent and stratigraphically similar Umbrella Point oil field. The result was idealized facies maps for three depositional settings: distributary channel, interdistributary bayfill (narrow channel and splays), and barrier bar. A total of 10 stochastic realizations were then created from each idealized facies map using TProGS (Transition Probability Geostatistics), a 3-D geostatistical simulation software package. Realizations for each layer of the final model were then selected, with different realizations of a particular facies being used for different layers.

Other modeling parameters were selected through examination of reservoir characteristics in similar facies in adjacent reservoirs. An injection rate of 0.75 million metric tons of CO_2 per well per year upon the injection rate in thicker, more permeable sands at Sliepner CO_2 injection project and an optimistic assessment of gas-production rates from Frio reservoirs. The numerical simulations were performed by using TOUGH2, a general-purpose simulator for multiphase flows in porous and fractured media.

A cutaway view of the TOUGH2 model created from the TProGS algorithm is shown in Figure 9 and the model results presented in figure 10 show CO_2 saturations at a series of times during the injection period. Preferential flow through higher permeability materials and buoyancy flow of the immiscible CO_2 are readily apparent.

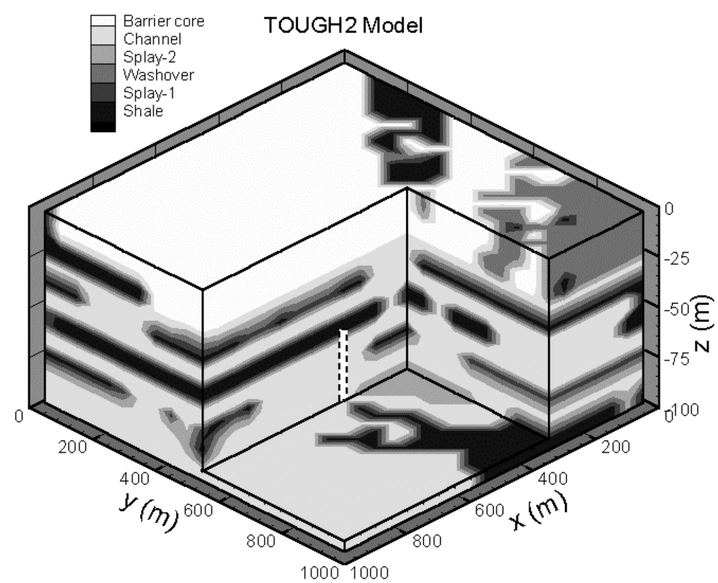

Figure 9. Probabilistically constrained facies for Baytown model with the injection interval in the lower half of the selected sand shown as a dashed box.

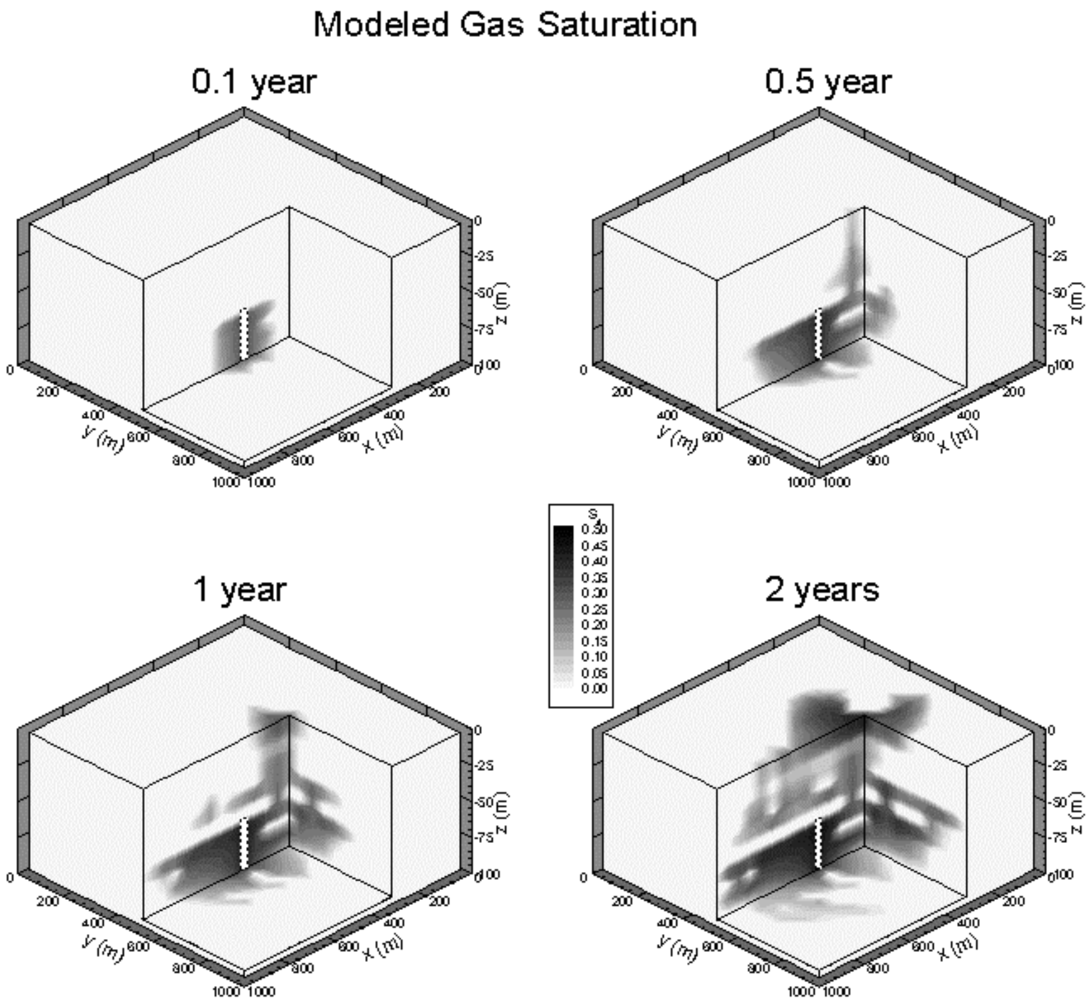

Figure 10. Simulated changes in CO_2 concentrations with time showing the effects of facies heterogeneity on geometry of the plume.

Work Next Quarter: Further study of the Frio Formation in the Baytown area will be carried out with models on three scales. Additional small-scale simulations will assess the effects of vertical and lateral heterogeneity on pressure buildup at CO_2 injection wells, the number of injection wells needed, and the influences of reservoir-scale heterogeneity on CO_2 storage efficiency. To move toward reservoir-scale simulations for assessing sequestration performance over a typical 30-year project lifetime, we will develop and test a conceptual model and modeling approach. Initial goals toward producing this reservoir-scale simulation include data compilation, experiments in methods of representing stratigraphically and structurally complex reservoirs in models grids, and testing the sensitivity of CO_2 behavior to these factors. Long-term (10,000-year) regional-scale simulations will assess how residence time is affected by CO_2 buoyancy, large-scale geological features, CO_2-brine interactions, and deep-basin brine migration. This simulation will be carried out by using a very narrow 3-dimensional grid that is aligned with buoyancy-driven movement of the CO_2 plume, but that still preserves some of the important characteristics of a 3-dimensional flow field. Creation of appropriate input data and initial model runs are goals for next quarter.